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October 1, 1993

Defense Technical Information Center
Building 5, Cameron Station
Alexandria, VA 22314

Dear Sir or Madam:

Re: GRANT N00014-93-1-2002

Enclosed please find a quarterly technical summary of the work performed at Colorado State University on the project titled "Materials Processing and Manufacturing Technologies for Diamond Substrate Multichip Modules (DSMCM)," for the period covering 1 July 1993 through 1 October 1993.

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Sincerely,

David S. Dandy
Assistant Professor
Chemical Engineering

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“Materials Processing and Manufacturing Technologies for Diamond Substrate Multichip Modules (DSMCM)”

Contract N00014-93-1-2002

David S. Dandy

Surface chemistry: Portions of a detailed surface kinetics mechanism—developed in collaboration with Michael Coltrin of Sandia National Laboratories—to describe the growth of diamond on a (100)-(2×1) surface have been refined extensively during this period. Specifically, it was discovered that the molecular mechanics program employed to calculate the thermophysical properties of the diamond structures was not parameterized for use with radical species. After discussions with the program's author (N.L. Allinger, Univ. Georgia, Athens) and extensive testing with experimentally validated compounds, MM3(92) has been re-applied to the 53 unique structures present in the surface mechanism to compute the temperature-dependent quantities enthalpy, entropy, and heat capacity for each structure. These thermodynamic properties have been fit to polynomials over the temperature range $298.15 \leq T \leq 2000$ K. The full mechanism is currently being incorporated into the stagnation flow model used to examine diamond deposition.

Pedestal Reactor Calculations: A suite of detailed experimental results for hot-filament and microwave assisted growth was provided by W.L. Hsu of Sandia; the results consist of molecular beam mass spectrometry measurements of neutral species concentrations in the boundary-layer above the diamond substrate. Stagnation flow calculations are underway to investigate the chemical differences arising from the use of a microwave plasma versus a glowing tungsten filament. In addition, the effect of using C_2H_2 instead of CH_4 as feed is being examined through the numerical calculations. Preliminary results confirm the speculation that gas-phase chemistry, particularly H_2 decomposition, cannot be explained as a purely thermal effect: unless heterogeneous chemistry occurs on the filament there is insufficient H present in the system to coincide with the mass spectrometry measurements.

Enclosed Reactor Calculations: A central issue controlling the success of enclosed reactor geometries will be the degree to which the gas in the reactor is well-mixed. By solving the exact momentum and thermal energy equations for specific reactor geometries, we can quantitatively measure the effectiveness of the hydrodynamic mixing (convective and diffusive) due to the motion of the jet issuing from a plasma gun. To this end a non-isothermal, multi-dimensional fluid dynamics code to analyze mixing effectiveness in enclosed reactors under the low pressure conditions used in diamond growth is under development and nearing readiness. Calculations are being performed on simple geometries under isothermal conditions to validate the code's accuracy. Simulations of flow under actual diamond growth conditions are scheduled to commence shortly.

Nucleation kinetics: After an initial dead end concerning a postdoctoral hire, a well-qualified candidate has been found. The individual is defending a PhD in nucleation kinetics and growth theory this month, and has begun to examine these issues as they pertain to the diamond system.

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